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Melting of ice simulated by a multicanonical method combined with a first-principles calculation YOSHIHIDE YOSHIMOTO, Department of Applied Mathematics and Physics, Graduate School of Engineering, Tottori University — Water is a ubiquitous material and is both scientifically and technologically important. For the simulation of water, the most common PBE semi-local exchange correlation (XC) functional has an issue: it gives over-structured liquid compared to the experimental one for a given temperature. On the other hand, the PBE0 hybrid XC functional was claimed to be better for the description of water recently [1,2]. In this study, the melting of ice, one of its most fundamental property, was simulated by a multicanonical method combined with a first-principles calculation [3,4]. Both the PBE XC functional and the PBE0 hybrid XC functional were adopted for the simulation. With accelerated computation of the hybrid functional by GPGPU, it was found that the PBE0 XC hybrid functional gave an improved melting temperature compared to that by PBE [5].

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Yoshihide Yoshimoto
Department of Applied Mathematics and Physics,
Graduate School of Engineering, Tottori University

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